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# Problem Set 2

- You may use your course materials and/or any literature resources (as well as the internet) to formulate your solutions.
- You may work in teams. However, each student must submit their individual work. *Solutions must be typed*. All model/analysis code must be submitted to GitHub and the link provided to the teaching staff for *each* student. Solutions should be submitted electronically to the teaching staff.
- Problem Set 2 is due on **Friday, March 31, 2017** by **4:59 PM**. Problem Set 2 is worth 100 points. A 50% penalty will be charged for each late day.

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1. (100 pts). **Reproduce W3110 Flux Balance Analysis (FBA) results.** Varma and Palsson used flux balance analysis (FBA) to estimate the specific growth rate, and the specific rates by-product formation for aerobic and anaerobic batch cultures of *Escherichia coli* W3110 grown on glucose (1). Reproduce the simulations in Fig. 7 and Fig. 11 of the Varma and Palsson study by conducting your own flux balance analysis. Strategy:

    a) (40 pts) Develop a stoichiometric model of W3110 central carbon metabolism (start with Palsson's website and Kegg). Use JuNQC (2) to transform your stoichiometric network model into a working Linear Program (LP).

    b) (20 pts) Test the correctness of your stoichiometric network by maximizing by-product formation (starting from glucose, in the presence of oxygen) for: (i) acetate, (ii) formate, (iii) ethanol and (iv) ATP. Confirm that your network is elementally balanced on C, O, P, N and H. (if not, why not?)

c) (10 pts) Reproduce the trends for Fig. 7. Plot your simulations versus the experimental data for Cellmass, glucose and acetate.

d) (10 pts) Reproduce the trends for Fig. 11. Plot your simulations versus the experimental data for Cellmass, glucose, acetate, ethanol and formate.

e) (20 pts) Explain the differences between the flux distribution predicted in Fig. 7 (aerobic growth on glucose) versus Fig. 11 (anaerobic growth on glucose)?

# References

1. Varma A, Palsson BO (1994) Stoichiometric flux balance models quantitatively predict growth and metabolic by-product secretion in wild-type escherichia coli w3110. Appl Environ Microbiol 60: 3724-31.

2. Varnerlab. https://github.com/varnerlab/JuNQC-Generator.